

Contaminant Permeation in the Ionomer-membrane Water Processor (IWP) System

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The Ionomer-membrane Water Processor (IWP) is a patented membrane-distillation based urine brine water recovery system. The unique properties of the IWP membrane pair limit contaminant permeation from the brine to the recovered water and purge gas. A paper study was conducted to predict volatile trace contaminant permeation in the IWP system. Testing of a large-scale IWP Engineering Development Unit (EDU) with urine brine pretreated with the International Space Station (ISS) pretreatment formulation was then conducted to collect air and water samples for quality analysis. Distillate water quality and purge air GC-MS results are presented and compared to predictions, along with implications for the IWP brine processing system.

Nomenclature

AES = Advanced Exploration Systems
ARC = Ames Research Center
ARFTA = Advanced Recycle Filter Tank Assembly
COTR = Contracting Officer Technical Representative
dP = delta Pressure
EDU = Engineering Development Unit
ePTFE = expanded Polytetrafluoroethylene
GC = Gas Chromatography
IC = Ion Chromatography
ICP-MS = Inductively Coupled Plasma Mass Spectrometry
ISS = International Space Station

IWP = Ionomer-membrane Water Processor
JSC = Johnson Space Center
LDL = Less than Detection Limit
MFSC = Marshall Space Flight Center
MS = Mass Spectrometry
NASA = National Aeronautics and Space Administration
SBIR = Small Business Innovative Research
SMAC = Spacecraft Maximum Allowable Concentration
TOC = Total Organic Carbon
UPA = Urine Processor Assembly
WFRD = Wiped-Film Rotating-Disk

I. Introduction

Closing the water loop on long duration spaceflight missions is a key aspect of reducing mission mass and logistics support for orbiting facilities and interplanetary spacecraft. Urine water recovery is currently restricted to the solubility limit of various compounds in pretreated urine such calcium phosphate, thus producing concentrated brine that requires further processing for water recovery. The Ionomer-membrane Water Processor (IWP) is a membrane-distillation based urine brine water recovery system. IWP operates open loop with cabin air and utilizes existing spacecraft systems such as the cabin-condensing heat exchanger and trace contaminant control system to minimize mass, volume, and complexity. The unique properties of the IWP membrane pair limit contaminant permeation from the brine to the recovered water, purge gas, and cabin atmosphere. The contaminant permeation dynamics of the IWP system are explored to evaluate its effectiveness at retaining trace contaminants. A paper study was conducted to predict volatile trace contaminant permeation in the IWP system. Testing of a large-scale IWP Engineering Development Unit (EDU) with urine brine pretreated with the International Space Station (ISS) pretreatment

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formulation was then conducted to collect air and water samples for quality analysis. Distillate water quality and purge air GC-MS results are presented and compared to predictions, along with implications for the IWP brine processing system.

A. Background

IWP is a patented dual-membrane distillation process. The first layer, a microporous membrane, allows bulk gas permeation at high rates while retaining the liquid and solids. The second layer is an ionomer membrane with selective permeability to water vapor. The ionomer transports water vapor while trapping harmful volatiles. Water vapor is swept away by a purge gas while residual dehydrated brine and volatiles are fully contained within the membranes. Because the membranes are extremely lightweight, the entire IWP membrane structure is disposable with the brine, maintaining brine containment throughout the life of processing and disposal. The consumable bladders are well within Advanced Exploration Systems (AES) exploration program goal of brine processing consumables mass of 25% or less of recovered water mass.¹ Figure 1 demonstrates the dehydrated urine containment in a disposable IWP bag after urine processing. The stages of brine processing from IWP testing are pictured in Figure 2, from original urine to pre-processed brine to recovered water.

The ionomer membrane baselined in the IWP technology is Nafion®, a copolymer of tetrafluoroethylene and perfluoro-3,6-dioxo-4-methyl-7-octene-sulfonic acid². Like Teflon, Nafion® is highly resistant to chemical attack, but the presence of its exposed sulfonic acid groups confers unusual properties. “Nafion® very readily absorbs water, from the vapor phase or from the liquid phase. Each sulfonic acid group will absorb up to 13 molecules of water. The sulfonic acid groups form ionic channels through the bulk hydrophobic polymer, and water is very readily transported through these channels. As such, Nafion® functions like a very selective, semi-permeable membrane to water vapor.”² This ability to selectively allow water to permeate suggests a possible role in water purification processes. The sulfonic acid groups pass water, but few other compounds, making it possible to separate water from a contaminated source.

The fact that Nafion® acts as an ion exchange resin when exposed to liquids suggests that Nafion® is most effective processing gases rather than liquid solutions. Solutions containing positive ions will reduce the effectiveness of Nafion®’s permeability function by approximately 66% by supplanting the hydrogen ions of the sulfonic acid group with that of the solution cations². As such, the Nafion®-based membrane pair solution is designed to deliver a vapor stream to the Nafion® surface; the ionomer is paired with a microporous membrane to prevent contamination of the ionomer.

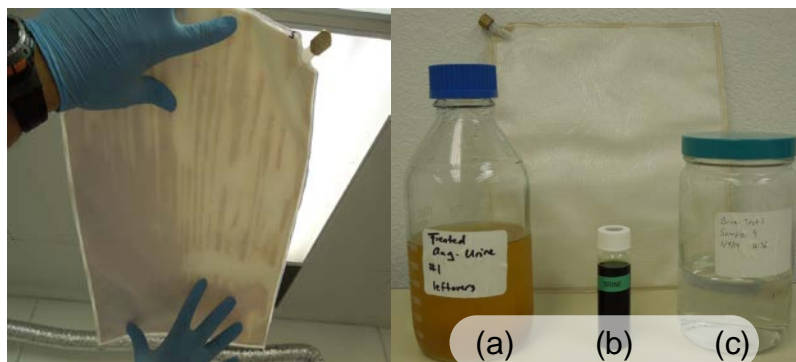


Figure 1: Final stage of urine bag with 98% of water removed; remaining material is “crunchy.” Figure 2: Stages of brine processing, original urine (a), pretreated urine brine (b), and extracted water (c).

II. Predicted Water and Air Quality

The IWP system utilizes cabin air as the sweep gas to move water vapor out of the IWP bladders, and vents into the cabin to take advantage of the cabin condensing heat exchanger to recover the water vapor. As some of the volatiles found in urine brine are hazardous to human health and equipment health, the safety of venting directly into the cabin must be taken into consideration. There are currently many compounds that off-gas during ISS Urine Processor Assembly (UPA) operations and vent into the cabin. This includes compounds such as methanol, ethanol, furan, trichloroethene, acetone and carbonyl sulfide.³ A similar understanding of trace contaminant loading from a brine processor must be established. As such, Paragon worked with Wyle Laboratories of Houston, TX to perform an independent evaluation of the volatile trace contaminant permeation in the IWP system.

The study began by determining potential concentrations of inorganic and organic components present in urine brine. The urine brine composition was compiled using data from brine and urine samples obtained from multiple ground tests at Johnson Space Center (JSC) and Marshall Space Flight Center (MSFC) operating under nominal UPA conditions. Once component concentrations were established, the compounds expected to volatilize and pass through the IWP membranes were evaluated. Due to the normal variability of urine, certain requirements and assumptions for the final brine composition were made:

1. Only inorganic components present in at least 2 of the 6 brine samples and with concentrations greater than 100 mg/L were compiled for final brine composition

- Only compounds present in at least 2 of the 8 preserved urine samples with concentrations of greater than 100 µg/L were further analyzed for potential brine composition
- A water recovery from urine of 75% by the UPA was assumed for the final brine concentration. Note that the concentrations of the volatile organic components in brine following greater water recovery (e.g. 85%) would be expected to be even lower due to further losses of the volatiles during distillation by the UPA.
- Volatile compounds and alcohols were assumed to be lost to the distillate on a 1:1 basis with water during UPA processing
- No losses to the distillate were assumed for non-volatile, semi-volatile, and ionic compounds
- Only inorganic compounds with final brine concentration of greater than 1000 µg/L were included in the final brine composition
- The data is based on sulfuric acid pretreated urine. Data for phosphoric acid-based pretreatment will be similar with the exception of increased phosphate and decreased sulfate.

Table 1 presents the expected organic components in brine based on the aforementioned requirements and assumptions. No inorganic compounds are expected to pass through the IWP membranes and so only organic compounds are further discussed. Because of the low pH of the brine (pH ~2), ammonia is not expected to volatilize in the system.

Table 1: Urine Brine Composition ⁴

Compound	Average Concentration in Preserved Urine (µg/L, 8 samples)	Predicted Concentration in Brine Following 75% Water Recovery (µg/L)
Volatiles/Alcohols		
Acetone	16,529	4,132
Acetaldehyde	4,621	1,155
Ethanol	15,791	3948
Methanol	4,809	1202
Semi-Volatiles		
Benzoic Acid	1,153	4,612
Benzyl Alcohol	312	1,247
Caffeine	1,959	7,835
Ibuprofen	1,231	4,926
Methyl Sulfone	8,385	33,538
Palmitic Acid	642	2,569
Phenol	613	2,452
2-Phenylacetic Acid	1,018	4,074
Salicylic acid	1,141	4,564
Vanillin	259	1,035
Acid Extractables		
4-Methylphenol	2,085	8,338
Carboxylates		
Formate	138,333	553,333
Non-Volatile		
Urea	16,492,500	65,970,000

Due to the dual-membrane nature of IWP, the ePTFE membrane retains all liquid and only allows vapor to pass. Thus, only compounds that are volatile at IWP operating conditions can pass through the ePTFE to reach the Nafion layer. The four compounds identified in the theoretical analysis performed by Wyle Laboratories are acetone, acetaldehyde, ethanol and

methanol. Of those, alcohols ethanol and methanol are expected to pass through Nafion. Due to the hydrophilic nature of Nafion conferred by the sulfonic acid groups, polar molecules such as alcohols are quickly absorbed by the membrane and would diffuse through to be removed by the purge gas. Ketones such as acetone may be converted to an alcohol via acid catalysis at the Nafion membrane and subsequently pass through the Nafion. Acetaldehyde is not known to be absorbed by Nafion.² Determining the transfer rates of the three compounds based on available literature is difficult. However, Nafion has the highest affinity towards water, with a decreasing order of affinity for methanol, isopropanol, and ethanol.⁵

Based on the average brine concentrations of Table 1, and assuming the 22 L of brine per processing batch from the Advanced Recycle Filter Tank Assembly (ARFTA), the total masses of acetone, ethanol, and methanol that could *potentially* transfer through the Nafion membrane are 91 mg, 87 mg, and 26 mg, respectively (Table 2). As a basis for comparison, using a representative Habitation Module free volume of 100 m³, the maximum concentrations of these three compounds in the module air would be 0.7, 0.6, and 0.2 mg/m³ if there was no removal by the trace contaminant control system. For reference, the interior volume of ISS is approximately 915 m³. A comparison with the Spacecraft Maximum Allowable Concentrations (SMAC) shows that none of these compounds approach the SMACs, even under worst case conditions of the volatile components of the brine being removed from the IWP as vapor and trapped in a single module.

Table 2: IWP Permeable Compound Quantities

Compound	Mass of Analyte in 22 L of brine (mg)	Worst Case Concentration* (mg/m ³)	180 day SMAC (mg/m ³)	100 day SMAC (mg/m ³)
Acetone	91	0.91	52	N/A
Ethanol	87	0.87	2000	2000
Methanol	26	0.26	90	30
Total	204			
* Assumption of dilution in 100 m ³ volume (typical ISS module)				

In reality, a trace contaminant control system (TCCS) would remove compounds from the cabin air. If all three compounds completely passed through the IWP membranes, the average contaminant loading over the course of an 11 day processing cycle is 0.77 mg/h. The TCCS aboard ISS is capable of removing trace contaminants at a rate of 230 mg/h.³ It is likely that any volatile permeation would not be an even rate over the course of processing, rather very high in the beginning. But as shown in the worst case scenario presented in Table 2 of no removal, the resulting concentrations would be well below SMAC. For an additional point of reference, Table 3 compares the potential IWP trace contaminant loading rate to a crew member's metabolic production rates.

Table 3: Predicted IWP Contaminants Maximum Permeation Rates

Compound	Mass of Analyte in 22 L of brine processed (mg/d)	METABOLIC (mg/person-d)
Acetone	6.15	19
Ethanol	5.88	4.3
Methanol	1.79	0.9
Total	13.82	24.8

In summary, a theoretical analysis of worst-case IWP trace contaminant production indicates that the IWP system is not expected to introduce hazardous levels of trace contaminants to the cabin environment or significant loading on the TCCS.

III. Measured Water and Air Quality

Extensive water and gas trace contaminant analyses were performed as part of the brine technology evaluation at Ames Research Center (ARC) during the summer of 2015. The test hardware and test setup are described below along with the results of the water and gas quality analyses.

A. EDU Description

The IWP EDU was developed to simulate the form, fit, and function of the IWP technology as applied in an ISS brine processor system design. The EDU consisted of two main parts: the brine bladder and housing. The bladder is constructed of the IWP microporous and ionomer membranes. It can hold up to 16.5L of brine, which is 75% of the 22L capacity of the ARFTA, and thus is considered a 75% full-scale brine processor for ISS. During operation, an empty bladder is installed into the housing. A fill port on the bladder is connected to a

feedthrough that passes through the housing wall to allow *in situ* filling of brine into the bladder. The housing provides containment of the bladder to direct and control the purge gas flow over the membrane surfaces. The purge gas enters one end of the housing and passes over the length of the brine bladder to promote water vapor permeation. The humid purge gas then exits the other end of the housing to be sampled and condensed. The housing is constructed of various types of plastic compatible with the brine as a precaution in the event of a leak during development testing. However, flight-rated materials of construction were not utilized and material off-gassing characteristics were not taken into consideration. The 75% of full-scale, IWP EDU is shown in Figure 3 and a bladder is shown in Figure 4. Support equipment for testing the EDU includes a heater and blower, plus a condenser to collect water samples, though a dedicated condenser is not part of the system design.

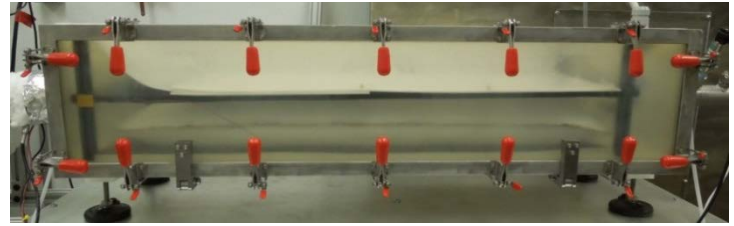


Figure 3: EDU for IWP System.



Figure 4: IWP EDU Bladder.

B. Test Description

The IWP EDU was delivered to Ames Research Center (ARC) in June 2014 for evaluation. The test bed schematic is shown in Figure 5 below. While the IWP has been operated in various configurations including open and closed loop, and gas sampling before and after the condenser, only the most recent test configuration from Summer 2015 testing is discussed in detail, as all test results presented in this paper are from the Summer 2015 testing. The IWP was run as an open system and vented to the fume hood using lab environment air as the carrier gas for evaporation of water from the membrane bag. The Ames lab environment air had a dew point temperature of $\sim 12.5^{\circ}\text{C}$.

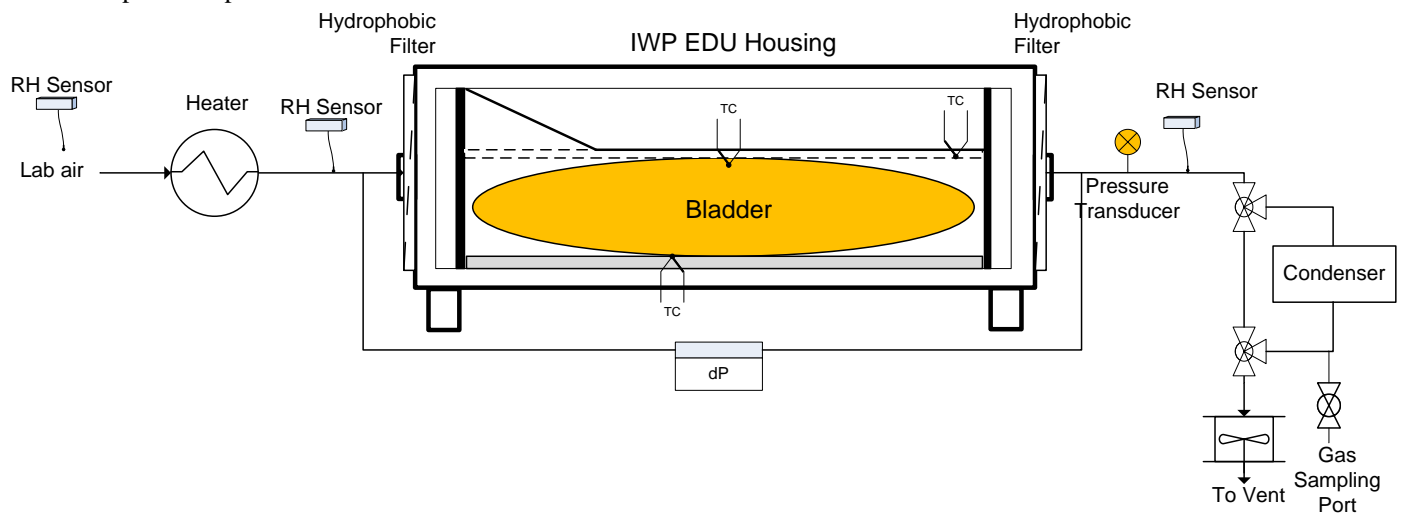


Figure 5: IWP EDU Test Bed Schematic

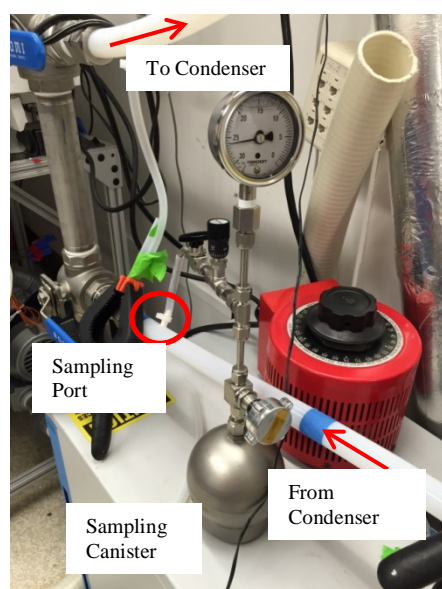


Figure 6: Gas Sample Collection Post-Condenser

The air flow was controlled by a variable frequency drive fan. The frequency set point was determined by flow bench testing at Paragon and pressure drop (dP) for the test bed associated with the flow was monitored during testing. The purge air flows through the heater before entering the EDU. Thermocouples inside the EDU monitor the temperature of the bladder and housing. A thermocouple located on the bladder surface was attached to the pre-EDU flow heater controller to maintain the brine temperature in the bladder. The purge gas exited the housing after picking up water vapor from the bladder. Pressure, temperature, and humidity of the purge stream were monitored before and after the EDU. A flow diverter feature in the EDU housing maintained the cross-sectional flow area and flow distribution as the brine bladder shrank from water removal during the course of testing. Gas and water condensate samples were collected for analysis. Gas samples were collected after the condenser, as shown in Figure 6. Because IWP operates open loop, a sample of the room air was taken simultaneously with the IWP vent gas sample.

During operation the bladder was filled with 12-16L of brine. A new bladder was used for each test. NASA Ames Research Center (ARC) provided brine for EDU testing. The wastewater brine was produced by removing 85% of the water from human urine. The urine was initially pretreated with the Alternative ISS urine pretreatment⁶ and salt concentrations adjusted to mimic astronaut urine.⁷ The brine was produced by processing urine in the Wiped-film Rotating-disk (WFRD) at ARC. The WFRD is a vapor compression distillation system used to simulate the ISS UPA function. The urine processed by the WFRD was collected from male volunteers at ARC.

C. Water and Air Quality Results

A comprehensive water quality analysis was performed by the Water Quality Laboratory at Johnson Space Center. The distillate composite sample was collected during the test run dated 9/22/2015. Only the compounds that were detected in the IWP distillate are presented in Table 4. A comprehensive listing of all compounds analyzed for and associated methods is found in the Appendix. Very few organic compounds were detected in the distillate. The Total Organic Carbons (TOC) concentration was measured as 42 mg/L.

The brine used for testing was not analyzed for direct comparison of contaminant reduction. In order to make a relative comparison, the brine analysis results from IWP EDU testing at Paragon in 2014 is shown in Table 5.⁸ Compared to average brine values, all compounds were reduced by over 99.9%. Sodium was 0.07 mg/L in the distillate, compared to more than 12,000 mg/L in brine. Ammonium was reduced from 2000 mg/L to 0.41 mg/L. Potassium decreased from ~15,000 mg/L to 0.1 mg/L. Calcium decreased from ~1600 mg/L to 0.03 mg/L. Finally, TOC was reduced from 50,000 mg/L to 42.3 mg/L. A small concentration of decamethylcycllopentasiloxane (D5) was also measured in the condensate.

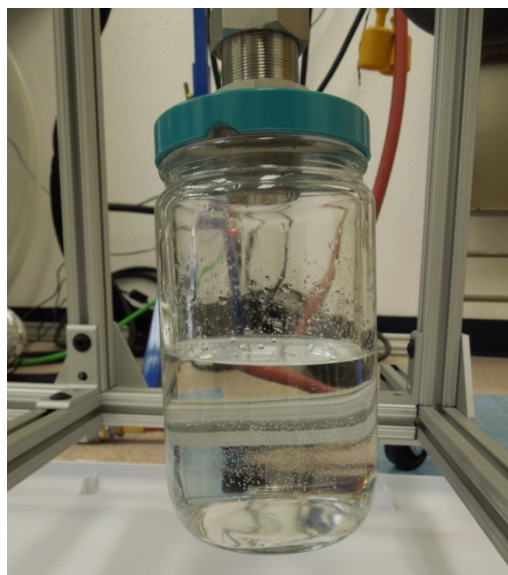


Figure 7: EDU Brine Testing Product Water Condensate

Table 4: Detected Compounds in IWP Distillate

Compound	Conc.	Compound	Conc.
Cations (IC)	mg/L	Volatiles (GC/MS)	µg/L
Ammonium (as N)	0.41	Acetone	293

Compound	Conc.	Compound	Conc.
Minerals (ICP-MS)	mg/L	Semi-volatiles (GC/MS)	µg/L
Calcium	0.03	Decamethylcyclopentasiloxane	5
Potassium	0.1	Methyl sulfone	196
Sodium	0.07	Semi-volatiles (GC/MS)	µg/L
Trace Metals (ICP-MS)	µg/L	2-Butoxyethanol	18
Aluminum	617	2-Ethylhexanoic acid	28
Chromium	35	Base/Neutral Extractables	µg/L
Iron	11,700	3,3-Dichlorobenzidine	NA
Manganese	122	bis-(2-Ethylhexyl)phthalate	13
Zinc	968	Benzyl alcohol	14
TOC (O.I.)	µg/L	Benzyl butyl phthalate	<4
NPOC	42,300	Dibutylphthalate	4
Acid Extractables	µg/L	Diethylphthalate	43
Benzoic acid	320		
Phenol	21		
4-Methylphenol	35		

Table 5: Representative Brine Composition from 2014 EDU testing at Paragon (units in mg/L)

Sample ID	Na+	NH4+	K+	Mg2+	Ca2+	Cl-	NO2-	Br-
Brine Feed 1	11022	1875	13817	592	1813	19764	LDL	LDL
Brine Feed 2	13678	2173	16753	443	1430	21544	LDL	LDL
Average	12350	2024	15285	518	1622	20654	LDL	LDL
Sample ID	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻	TOC	pH	Cond (µS)	Cr, hexavalent	Cr, trivalent
Brine Feed 1	LDL	100739	15089	49500	2.6	225000	<0.50	5730
Brine Feed 2	LDL	101083	14885	51760	2.6	229000	<0.50	4560
Average	LDL	100911	14987	50630	2.6	227000	<0.50	5145



Figure 8: Condenser Fitting Rusting

Large concentrations of trace metals were detected in the processed water condensate. These metals came from the non-flight like condenser and downstream fittings and components that were utilized during testing. The heat exchanger itself was made of aluminum. Downstream ducting and fittings were made of both galvanized steel and stainless steel. Chromium, iron, manganese, and zinc are all found in various forms of steel. Manganese and chromium are part of alloy steel. Zinc is used in electroplating galvanized steel, which was used in a duct after the condenser. Protective plastic sheeting was used in an attempt to prevent liquid contact with the steel and aluminum components. However, upon condenser disassembly after all testing was completed, it was found that the plastic layer became displaced and water was allowed to pool at a fitting, causing corrosion and leaching the metal compounds in the condensate (see Figure 8). When the condenser was originally assembled, it was only intended to be used for a period of weeks to a few months as part of a Phase II SBIR, and thus more temporary, cost-effective solutions were sought. Future

ground testing development work will utilize a higher-fidelity condensing heat exchanger for gathering condensate samples.

The results of the purge gas trace contaminants analysis are presented in Table 6. Again, only detected compounds are shown here. The comprehensive listing of all compounds included in the analysis is found in the Appendix. Gas samples were collected in Summa canisters and GC and GC/MS analyses were performed by Wyle Laboratories of Houston, TX. Gas samples were collected from the room air (inlet air to IWP) and IWP vent gas after the condenser during the 9/22/15 brine test run.

Table 6: Detected Trace Contaminants in Purge Gas⁹

Target Compounds	Ames IWP Room Air (mg/m ³)	Ames IWP Process (mg/m ³)	IWP TC Load (mg/m ³)
Ethanol	TRACE	<0.045	N/A
Methanol	TRACE	TRACE	TRACE
Acetaldehyde	0.063	0.094	0.031
Acetone	0.056	0.25	0.194
Octamethylcyclotetrasiloxane (D ₄)	TRACE	0.52	0.52
Decamethylcyclopentasiloxane (D ₅)	1.2	1.1	-0.1
Hexamethylcyclotrisiloxane (D ₃)	1.2	0.56	-0.64
Total Alcohols plus Acetone	0.081	0.27	0.189
Total Concentration (Non-Methane Hydrocarbons)	3.0	2.6	-0.4

Only three contaminants—acetaldehyde, acetone, and octamethylcyclotetrasiloxane (D₄ siloxane)—were detected downstream of the test rig condenser. These contaminants overlay a spacecraft's basic trace contaminant load from equipment offgassing and crew metabolism. Using the EDU flow rate and assuming a constant generation rate, the three compounds combined increase the spacecraft trace contaminant control system loading by ~22 mg/hr.¹⁰ For ISS, this represents a 3.5% increase to the total ISS trace contaminants generation rate of 587 mg/hr,^{11,12} resulting in an ECLSS compatibility rating of E1 Minor for the IWP purge gas when contaminant loading is taken as a whole.¹³ For an exploration mission with 4 crew members and a 280 m³ pressurized volume (approximate midpoint between an Ideal volume and Aggressive volume¹⁴), the 22 mg/hr IWP trace contaminant generation rate represents a 38% increase in the spacecraft hourly generation rate.¹⁵ This translates to an ECLSS compatibility rating of E3 Moderate for an exploration craft. ECLSS compatibility ratings were determined using the overall trace contaminant control system load as the impact. Evaluating compounds individually helps to understand the primary drivers for the overall impact rating. For example, the acetone production rate from IWP would be 5.8 mg/hr, a 37% increase to the current 15.75 mg/hr station load. The IWP generation rate of acetaldehyde is 0.93 mg/hr, 8.8% of the station acetaldehyde load of 10.54 mg/hr. The largest contribution to the total trace contaminant increased loading from IWP is the D₄ siloxane. The IWP EDU generation rate of D₄ siloxane is 15.2 mg/hr, which represents an 18% increase in the overall siloxanes (D₃, D₄, D₅) station load of 83.7 mg/hr. From this assessment, although the D₄ siloxane presents the greatest overall IWP trace contaminant load component, the acetone load component is the primary driver for ECLSS compatibility impact. The IWP trace contaminant generation rates are estimated assuming a worst case of continuous, maximum concentrations. Actual concentrations may be intermittent which may result in a lower overall trace contaminant loading impact.

While acetone and acetaldehyde are found in brine, the siloxane is likely due to offgassing from plastics used in the EDU. While it may not be practical to eliminate D₄ offgassing completely since siloxanes are generated by many types of plastics, careful material selection and avoidance of silicone for a flight design may reduce the siloxane off-gassing from IWP. For use aboard the ISS, a point-of-use trace contaminant control capability may not be necessary for the IWP vent gas given the minor impact to the overall ISS trace contaminant loading. However, a source control activated carbon trace contaminant scrubber may be needed for an exploration mission. Although D₄ siloxane was the largest component of the IWP contaminant load, acetaldehyde is actually the most difficult to capture with activated carbon, having an equilibrium adsorption capacity that is 80 times lower than acetone and over two orders of magnitude lower than cyclic siloxanes and would thus drive the local trace contaminant control scrubber sizing, though the consumables rate would be driven by the siloxane.¹⁶

Gas samples were collected after the condenser so that test data could be directly compared to competing brine processing systems. Sample collection limitations associated with the competing systems drove the sampling location. Unfortunately, this sampling location is neither directly representative of the IWP operational concept nor does it reflect the complete impact of the IWP purge gas composition to the cabin environment. The IWP does not include a dedicated condenser and vents the humidified purge gas directly to the cabin. Thus, a higher contaminant load is likely in the IWP purge gas than was measured. This load, when vented to the cabin, overlays the basic cabin trace contaminant load that is handled by the trace contaminant control system

and may increase the contaminant load in humidity condensate that is fed the water processor. The most representative gas sample should ideally be collected upstream of the condenser as some compounds may absorb in the condensate according to Henry's law, altering the load in the gas phase. Additional testing and process gas composition analysis is required to more definitively characterize the IWP's impact to the cabin environment.

Conducting a material balance around the test rig condenser allows for the total process gas trace contaminant load in the 30 m³/h sweep gas flow to be determined. Over the course of the experimental run, 7.15 L of water was recovered by the test rig's condenser in 144 hours, which yields a time-averaged 0.05 L/h collection rate. Based on the sweep gas flow, water collection rate conditions, and the 8.6°C condenser temperature, the Henry's Law-based calculation techniques presented by Perry¹² were used to determine a total gas phase trace contaminant loading the IWP sweep gas. Any background contributions were subtracted as appropriate to determine the net concentration load present in the IWP sweep gas that can be fully attributed to the IWP. Table 7 provides the total gas loading in order of highest to lowest concentration. Siloxanes, acetone, and acetaldehyde are the dominant compounds. On evaluating the additional load from compounds in the condensate for ECLS compatibility, the initial ECLS compatibility assessment ratings are still valid based on this analysis. Collecting process gas samples upstream of the condenser during future tests will validate this assessment.

Table 7: Process Gas Trace Contaminant Loading

Compound	Concentration (mg/m ³)
Octamethylcyclotetrasiloxane (D4)	0.51
Acetone	0.26
Decamethylcyclopentasiloxane (D5)	0.23
Acetaldehyde	0.031
Bis-(2-ethylhexyl)phthalate	0.0026
Ammonia	0.001
2-ethylhexanoic acid	0.001
4-methylphenol	0.00033
2-butoxyethanol	0.00012
Phenol	0.00011
Benzoic acid	0.00064
Diethylphthalate	0.00056
Methyl sulfone	0.00048
Benzyl alcohol	0.000041
Dibutylphthalate	0.000028

IV. Discussion

From the study to predict contaminant volatilization and permeation through IWP, acetone, methanol, ethanol, and acetaldehyde were predicted to volatilize from the brine at the IWP conditions and pass through the microporous membrane to come into contact with the Nafion. Of those four compounds, acetone, methanol, and ethanol were predicted to transfer through Nafion to end up in the air stream. Acetone was found in both the distillate condensate and vent gas sample. Ethanol was not detected in either the condensate or the vent gas. Methanol was not found in the condensate, and only a trace amount was detected in the vent gas, though a trace amount was already in the room air. While methanol and ethanol both can permeate through Nafion, the affinity of Nafion to water is much higher. It is possible that in the presence of abundant water vapor, the water vapor preferentially reacted to and passed through the Nafion, leaving few sites for methanol or ethanol to utilize for transfer.

Acetaldehyde was not expected to transfer through Nafion. As a class, aldehydes are converted to alcohols by Nafion. However, smaller aldehydes, such as formaldehyde and acetaldehyde, are resistant to enolization, and they are not absorbed by the Nafion. In fact, the distributor of Nafion driers indicates that no acetaldehyde is removed by their membranes.² But acetaldehyde is highly miscible in water. Experience has shown that certain highly water soluble gases can transfer through Nafion in the presence of water, that in a dry environment would otherwise not react with or pass through Nafion.^{2,17} Water permeates through Nafion by first binding to an exposed sulfonic acid group on the surface of the membrane. The water then permeates through the membrane by being transferred rapidly from sulfonic acid to adjoining sulfonic acid. Finally, the water pervaporates from a bound solid state directly to the vapor phase in the surrounding gas. It is speculated that after the water molecule initially binds to the exposed sulfonic acid site, highly water-soluble gases may bind to the water molecule while it is

still exposed on the surface of the membrane and remain bound as the water molecule permeates through the Nafion.² Formaldehyde is found to transfer through Nafion in this fashion. It is suspected that acetaldehyde can as well, which would account for its presence in the distillate.

V. Conclusion

The IWP distillate was demonstrated to have very few brine contaminants in either the condensate or vent gas. The high water quality would not impose a significant load to the ISS Water Processor Assembly. Siloxane, likely from the plastics used in the EDU, was found in the vent gas, though siloxane contamination also presents major challenges in trace analysis as they are brought into laboratories in personal care products and are essential components in laboratory equipment.¹⁸ The three compounds detected in the vent gas combined increase the spacecraft trace contaminant control system loading by ~22 mg/hr, a 3.5% increase to the total ISS trace contaminant generation rate, resulting in an ECLSS compatibility rating of E1 Minor. A point-of-use trace contaminant control capability may not be necessary for the IWP vent gas given the minor impact to the overall ISS trace contaminant loading. However, a source control activated carbon trace contaminant scrubber may be needed for an exploration mission, where the 22 mg/hr IWP trace contaminant generation rate represents a 38% increase in the spacecraft hourly generation rate, translating to an ECLSS compatibility rating of E3 Moderate. Sampling of the gas composition prior to the condenser for toxic hazard analysis by NASA toxicologists is planned for future work, though a preliminary comparison between distillate and gas contaminant concentrations suggests that the loss of contaminants during condensation was small, such that the existing data may be representative of a flight application of an IWP brine processor assembly.

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VI. Appendix

Table 8: Comprehensive Condensate Water Quality Analysis

Cations (IC)	mg/L	Volatiles (P&T/GC/MS)	µg/L	Volatiles (P&T/GC/MS)	µg/L	Volatiles (P&T/GC/MS)	µg/L
Ammonium(asN)	0.41	Acetone	293	Dichlorodifluoromethane	<50	Pentachloroethane	<50
Total S (ICP-MS)	mg/L	Acrylonitrile	<50	1,1-Dichloroethane	<50	Propionitrile (Ethyl cyanide)	<50
Total S	Pending	Allyl chloride (3-Chloropropene)	<50	1,2-Dichloroethane	<50	n-Propylbenzene	<50
Minerals (ICP-MS)	mg/L	Benzene	<50	1,1-Dichloroethene	<50	Styrene	<50
Calcium	0.03	Bromobenzene	<50	cis-1,2-Dichloroethene	<50	1,1,1,2-Tetrachloroethane	<50
Magnesium	<0.01	Bromochloromethane	<50	trans-1,2-Dichloroethene	<50	1,1,2,2-Tetrachloroethane	<50
Phosphate(asP)	<0.01	Bromodichloromethane	<50	1,2-Dichloropropane	<50	Tetrachloroethene	<50
Potassium	0.1	Bromoform	<50	1,3-Dichloropropane	<50	Tetrahydrofuran	<50
Sodium	0.07	Bromomethane	<50	2,2-Dichloropropane	<50	Toluene	<50
Trace Metals (ICP-MS)	µg/L	2-Butanone (Methyl ethyl ketone)	<50	1,1-Dichloropropanone	<100	1,2,3-Trichlorobenzene	<50
Aluminum	617	n-Butylbenzene	<50	1,1-Dichloropropene	<50	1,2,4-Trichlorobenzene	<50
Antimony	<4	sec-Butylbenzene	<50	cis-1,3-Dichloropropene	<50	1,1,1-Trichloroethane	<50
Arsenic	<2	tert-Butylbenzene	<50	trans-1,3-Dichloropropene	<50	1,1,2-Trichloroethane	<50
Barium	<2	Carbon disulfide	<50	Diethyl ether	<50	Trichloroethene	<50
Beryllium	<2	Carbon tetrachloride	<50	Ethylbenzene	<50	Trichlorofluoromethane	<50
Cadmium	<2	Chloroacetonitrile	<100	Ethyl methacrylate	<50	1,2,3-Trichloropropane	<50
Chromium	35	Chlorobenzene	<50	Hexachlorobutadiene	<50	1,2,4-Trimethylbenzene	<50
Cobalt	<2	1-Chlorobutane (Butyl chloride)	<50	Hexachloroethane	<50	1,3,5-Trimethylbenzene	<50
Copper	<2	Chloroethane	<50	2-Hexanone	<50	Vinyl Acetate	<50
Iron	11,700	Chloroform	<50	Iodomethane	<50	Vinyl Chloride	<50
Lead	<2	Chloromethane	<50	Isopropylbenzene (Cumene)	<50	m & p-Xylene	<100
Manganese	122	2-Chlorotoluene	<50	4-Isopropyltoluene (Cymene)	<50	o-Xylene	<50
Mercury	Pending	4-Chlorotoluene	<50	Methacrylonitrile	<50	Volatiles (GC/MS)	µg/L
Molybdenum	<2	Dibromochloromethane	<50	Methyl acrylate	<50	Acetaldehyde	not found
Nickel	<2	1,2-Dibromo-3-chloropropane	<50	Methyl-t-butyl ether (MTBE)	<50	Trimethylsilanol	not found
Selenium	<2	1,2-Dibromoethane (EDB)	<50	Methylene chloride (Dichloromethane)	<50	Volatiles - Non-Targets (GC/MS)	µg/L
Silver	<2	Dibromomethane	<50	Methyl methacrylate	<50	Methyl disulfide	not found
Zinc	968	1,2-Dichlorobenzene	<50	4-Methyl-2-pentanone	<50	Semi-volatiles (GC/MS)	µg/L
TOC (O.I.)	µg/L	1,3-Dichlorobenzene	<50	Naphthalene	<50	Benzothiazole	<4
NPOC	42,300	1,4-Dichlorobenzene	<50	Nitrobenzene	<50	N-n-Butylbenzenesulfonamide	<4
		trans-1,4-Dichloro-2-butene	<50	2-Nitropropane	<50	Tris(2-Chloroethyl)phosphate	<10

Semi-volatiles (GC/MS)	µg/L	Base/Neutral Extractables	µg/L	Base/Neutral Extractables	µg/L	Semi-volatiles (GC/MS)	µg/L	Alcohols/Acetone	µg/L
Decamethylcyclotrisiloxane	5	N-Nitrosodi-n-propylamine	<8	Hexachlorobutadiene	<8	2-Mercaptobenzothiazole	not found	3-Methyl-1-butanol (Isopentanol)	<400
Dodecamethylcyclotetrasiloxane	<4	2,4-Dinitrotoluene	<8	Hexachlorocyclopentadiene	<8	2-Methyl-2,4-pentanediol	not found	2-Methyl-1-propanol	NA
bis-(2-Ethylhexyl) adipate	<4	2,6-Dinitrotoluene	<8	Hexachloroethane	<8	1-Methyl-2-pyrrolidinone	not found	2-Methyl-2-propanol	NA
Methyl sulfone	196	Isophorone	<4	1,2,4-Trichlorobenzene	<8	Methyl 4-hydroxybenzoate	not found	1-Pentanol (Amyl alcohol)	<400
2-Methylthiobenzothiazole	<4	Nitrobenzene	<8	Benzidine	NA	2-Methyl butyric acid	not found	2-Pentanol (sec-Amyl alcohol)	<400
Octamethylcyclotetrasiloxane	<4	Acenaphthene	<8	N-Nitrosodimethylamine	<8	Monomethyl phthalate	not found	3-Pentanol	<400
Acid Extractables	µg/L	Acenaphthylene	<8	N-Nitrosodiphenylamine	<8	(+)-Neomenthol	not found	1-Propanol	<400
Benzoic acid	320	Anthracene	<8	Semi-volatiles (GC/MS)	µg/L	Nicotine	not found	2-Propanol	<400
4-Chloro-3-methylphenol	<8	Benzo(a)anthracene	<8	Acetophenone	not found	Nonanoic acid	not found	Non-volatiles (LC/UV-VIS)	µg/L
2-Chlorophenol	<8	Benzo(a)pyrene	<5	Benzaldehyde	not found	Oxindole	not found	Urea	<800
2,4-Dichlorophenol	<8	Benzo(b)fluoranthene	<4	2-Butoxyethanol	18	Palmitic acid	not found		
2,4-Dimethylphenol	<8	Benzo(ghi)perylene	<5	2-(2-Butoxyethoxy)ethanol	not found	2-Phenoxyethanol	not found		
2,4-Dinitrophenol	<8	Benzo(k)fluoranthene	<4	Butylated hydroxyanisole (BHA)	not found	N-Phenyl-2-naphthylamine	not found		
2-Methyl-4,6-dinitrophenol	<8	Chrysene	<10	3-tert-Butylphenol	not found	2-Phenyl-2-propanol	not found		
2-Nitrophenol	<8	Dibenzo(a,h)anthracene	<5	Caffeine	not found	2-Phenylacetic acid	not found		
4-Nitrophenol	<8	Fluoranthene	<4	Dibutylamine	not found	Phenethyl alcohol	not found		
Pentachlorophenol	<8	Fluorene	<8	Diethylene glycol monoethyl ether	not found	Salicylic acid	not found		
Phenol	21	Indeno(1,2,3-cd)pyrene	<5	N,N-Diethylformamide	not found	Tetramethyl thiourea	not found		
2,4,6-Trichlorophenol	<8	Naphthalene	<20	N,N-Dimethyl acetamide	not found	Thymol	not found		
o-Cresol (2-Methylphenol)	<4	Phenanthrene	<4	N,N-Dimethylbenzylamine	not found	1,3,5-Triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	not found		
4-Methylphenol	35	Pyrene	<4	N,N-Dimethylformamide	not found	Tributylamine	not found		
2,4,5-Trichlorophenol	<8	bis(2-Chloroethyl) ether	<8	Dipropylene glycol methyl ether	not found	Tributyl phosphate	not found		
Base/Neutral Extractables	µg/L	bis(2-Chloroethoxy) methane	<8	2-Ethoxyethanol	not found	Triethyl phosphate	not found		
3,3-Dichlorobenzidine	NA	bis(2-Chloroisopropyl) ether	<8	2-Ethyl-1-hexanol	not found	Vanillin	not found		
bis-(2-Ethylhexyl)phthalate	13	4-Bromophenyl phenyl ether	<8	2-Ethylhexanoic acid	28	Alcohols/Acetone	µg/L		
Benzyl alcohol	14	4-Chlorophenyl phenyl ether	<8	4-Ethylmorpholine	not found	1-Butanol	<400		
Benzyl butyl phthalate	<4	2-Chloronaphthalene	<8	Heptanoic acid	not found	2-Butanol	<400		
Dibutylphthalate	4	1,2-Dichlorobenzene	<8	Hexanoic acid	not found	Ethanol	<400		
Diethylphthalate	43	1,3-Dichlorobenzene	<8	2-Hydroxybenzothiazole	not found	Methanol	<400		
Dimethylphthalate	<4	1,4-Dichlorobenzene	<8	Ibuprofen	not found	2-Methyl-1-butanol	<400		
Di-n-octyl phthalate	<8	Hexachlorobenzene	<8	p-Menth-1-en-8-ol (alpha-Terpineol)	not found	2-Methyl-2-butanol	NA		

Table 9: Comprehensive Vent Gas Trace Contaminants Analysis

CHEMICAL CONTAMINANT	AA05977 S/N 21260 AMES IWP ROOM AIR 9/22/2015	AA05978 S/N 22377 AMES IWP PROCESS 9/22/2015		AA05977 S/N 21260 AMES IWP ROOM AIR 9/22/2015	AA05978 S/N 22377 AMES IWP PROCESS 9/22/2015
TARGET COMPOUNDS (T0-15) **			2-Butenal	<0.025	<0.045
Freon 12 (Dichlorodifluoromethane)	TRACE	<0.045	1,2-Dichloroethane	<0.025	<0.045
Chloromethane	<0.025	<0.045	1,1,1-Trichloroethane	<0.025	<0.045
Freon 114 (1,2-Dichloro-1,1,2,2-tetrafluoroethane)	<0.025	<0.045	1-Butanol	<0.025	<0.045
Methanol	TRACE	TRACE	Benzene	<0.025	<0.045
Acetaldehyde	0.063	0.094	Carbon Tetrachloride	<0.025	<0.045
Vinyl Chloride	<0.025	<0.045	2-Pentanone	<0.025	<0.045
Bromomethane	<0.025	<0.045	2-Methylhexane	<0.025	<0.045
Ethanol	TRACE	<0.045	2,3-Dimethylpentane	<0.025	<0.045
Chloroethane	<0.025	<0.045	Pentanal	<0.025	<0.045
Acetonitrile	<0.025	<0.045	3-Methylhexane	<0.025	<0.045
Propenal (Acrolein)	<0.025	<0.045	1,2-Dichloropropane	<0.025	<0.045
Acetone *	0.056	0.25	1,4-Dioxane	<0.025	<0.045
Propanal (Propionaldehyde) #	<0.025	TRACE	Trichloroethene	<0.025	<0.045
2-Propanol (Isopropanol)	<0.025	<0.045	2,5-Dimethylfuran	<0.025	<0.045
Freon 11 (Trichlorofluoromethane)	<0.025	<0.045	n-Heptane	<0.025	<0.045
Furan	<0.025	<0.045	4-Methyl-2-pentanone (MIBK)	<0.025	<0.045
Acrylonitrile	<0.025	<0.045	cis-1,3-Dichloropropene	<0.025	<0.045
Pentane	<0.025	<0.045	2-Pentenal	<0.025	<0.045
2-Methyl-2-propanol	<0.025	<0.045	trans-1,3-Dichloropropene	<0.025	<0.045
Methyl acetate	<0.025	<0.045	1,1,2-Trichloroethane	<0.025	<0.045
1,1-Dichloroethene	<0.025	<0.045	Toluene	<0.025	<0.045
Methylene chloride (Dichloromethane)	<0.025	<0.045	Hexanal	<0.025	<0.045
3-Chloropropene (Allyl chloride)	<0.025	<0.045	Mesityl oxide (4-Methyl-3-penten-2-one)	<0.025	<0.045
Freon 113 (1,1,2-Trichloro-1,2,2-trifluoroethane)	<0.025	<0.045	1,2-Dibromoethane (EDB)	<0.025	<0.045
1-Propanol	<0.025	<0.045	Butyl acetate	<0.025	<0.045
1,1-Dichloroethane	<0.025	<0.045	Octane	<0.025	<0.045
Butanal (Butyraldehyde)	<0.025	<0.045	Tetrachloroethene (Perchloroethene)	<0.025	<0.045
2-Butanone (Methyl ethyl ketone)	<0.025	<0.045	Chlorobenzene	<0.025	<0.045
cis-1,2-Dichloroethene	<0.025	<0.045	Ethylbenzene	<0.025	<0.045
2-Methylfuran	<0.025	<0.045	m & p-Xylene	<0.050	<0.090
Ethyl acetate	<0.025	<0.045	2-Heptanone	<0.025	<0.045
Hexane	<0.025	<0.045	Cyclohexanone	<0.025	<0.045
Chloroform	<0.025	<0.045	Heptanal	<0.025	<0.045

CHEMICAL CONTAMINANT	AA05977 S/N 21260 AMES IWP ROOM AIR 9/22/2015	AA05978 S/N 22377 AMES IWP PROCESS 9/22/2015
1,1,2,2-Tetrachloroethane	<0.025	<0.045
o-Xylene	<0.025	<0.045
Nonane	<0.025	<0.045
1,3,5-Trimethylbenzene	<0.025	<0.045
1,2,4-Trimethylbenzene	<0.025	<0.045
1,3-Dichlorobenzene	<0.025	<0.045
1,4-Dichlorobenzene	<0.025	<0.045
1,2-Dichlorobenzene	<0.025	<0.045
1,2,4-Trichlorobenzene	<0.050	<0.090
Hexachlorobutadiene	<0.075	<0.13
Octafluoropropane (Perfluoropropane)	<0.10	<0.18
Perfluoro(2-methylpentane)	<0.050	<0.090
Carbonyl sulfide (Carbon oxide sulfide)	<0.025	<0.045
Isobutane	<0.025	<0.045
2-Methyl-1-propene	<0.025	<0.045
Dimethyl sulfide	<0.025	<0.045
Carbon disulfide	<0.025	<0.045
Trimethylsilanol	TRACE	<0.045
Octamethylcyclotetrasiloxane	TRACE	0.52
Decamethylcyclopentasiloxane	1.2	1.1
Propene	<0.050	<0.090
Propane	<0.050	<0.090
1,3-Butadiene	<0.050	<0.090
Butane	<0.050	<0.090
Isoprene (2-Methyl-1,3-butadiene)	<0.050	<0.090
SPECIAL INTEREST COMPOUNDS ***		
Ethylene oxide	<0.050	<0.090
2-Methyl-2-propenal	<0.050	<0.090
3-Buten-2-one	<0.050	<0.090
2-Ethoxyethanol	<0.050	<0.090
Dimethyl Disulfide	<0.050	<0.090
Hexamethylcyclotrisiloxane \$	1.2	0.56
NON-TARGET COMPOUNDS ***		
Formaldehyde \$\$	<0.060	<0.11
1,3-Pentadiene	<0.050	<0.090
3-Methyl-2-butanone	<0.050	<0.090
Allyl methyl sulfide	<0.050	<0.090
2-Ethylfuran	<0.050	<0.090
Methyl 2-propenyl disulfide	<0.050	<0.090
Octanal	<0.050	<0.090
Carbon monoxide **	0.43	<0.41
TOTAL ALCOHOLS PLUS ACETONE		
	0.081	0.27

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